Crystal Structure Solution of Organic Compounds by Simulated Annealing	X3B1

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The high resolution X-ray powder diffraction patterns of the compounds (I)2-amino-4,5-dimethoxyacetophenone, (II)1,4-benzenedimethanol and (III)3-aminoquinoline, were collected at the SUNY X3B1 beamline. They were indexed using the programs ITO and TREOR. Space groups were assigned based in the systematic absences and Z values of 4 were estimated from measured densities. The integrated intensities obtained after Le Bail fits using the program FULLPROF, together with the space group symmetry, cell parameters and cartesian coordinates for the molecules were entered to a program applying the simulated annealing algorithm, minimizing the difference between the calculated and observed integrated intensities. Possible crystal structure solutions in the direct space are generated assigning random numbers to the position (three coordinates) and orientation (three Eulerian angles) of rigid fragments in the unit cell. Additional numerical parameters areneeded for the conformational degrees of freedom (torsional angles in I and II).Final Rietveld refinements were done with the program GSAS, in which the atomic coordinates were subject to rigid body constrains. Figure 1 shows the crystal structure of (III).

[1]-E. Aarts and J. Korst, Simulated Annealing and Boltzmann Machines, J. Wiley and Sons, New York (1989).

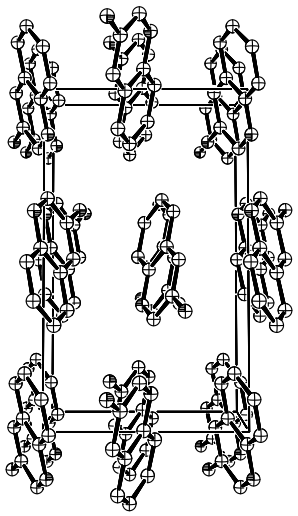

Figure 1. Crystal structure of 3-aminoquinoline view along the [001] direction. Hydrogen atoms are not shown.